

10/562,490 11/7/2006

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'CASREACT' ENTERED AT 16:13:55 ON 06 NOV 2006
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FILE CONTENT:1840 - 30 Oct 2006 VOL 145 ISS 18

New CAS Information Use Policies, enter HELP USAGETERMS for details.

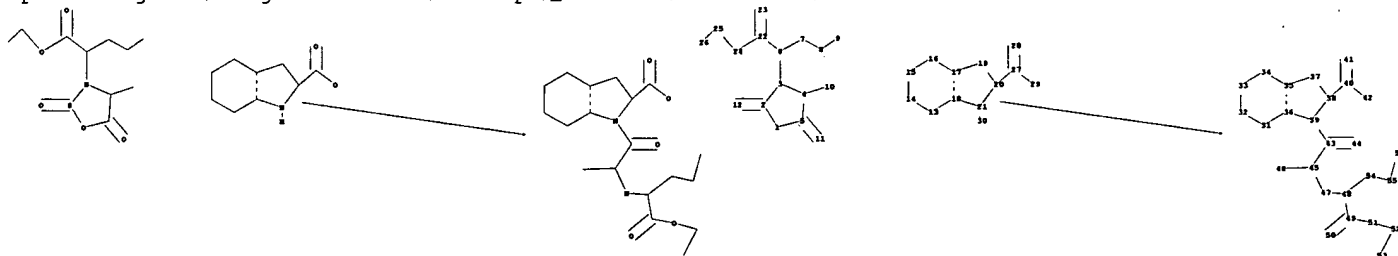
*
* CASREACT now has more than 10 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

Uploading C:\Program Files\Stnexp\Queries\10562490\IV+V.VI.str



chain nodes :

6 7 8 9 10 11 12 22 23 24 25 26 27 28 29 30 40 41 42 43 44 45 46
47 48 49 50 51 52 53 54 55 56

ring nodes :

1 2 3 4 5 13 14 15 16 17 18 19 20 21 31 32 33 34 35 36 37 38 39

chain bonds :

2-12 3-6 4-10 5-11 6-7 6-22 7-8 8-9 20-27 21-30 22-23 22-24 24-25 25-26
27-28 27-29 38-40 39-43 40-41 40-42 43-44 43-45 45-46 45-47 47-48 48-49 48-54
49-50 49-51 51-52 52-53 54-55 55-56

ring bonds :

1-2 1-5 2-3 3-4 4-5 13-14 13-18 14-15 15-16 16-17 17-18 17-19 18-21 19-20
20-21 31-32 31-36 32-33 33-34 34-35 35-36 35-37 36-39 37-38 38-39

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exact/norm bonds :

1-2 1-5 2-3 2-12 3-4 3-6 4-5 5-11 13-14 13-18 14-15 15-16 16-17 17-18 17-19
18-21 19-20 20-21 22-23 22-24 24-25 27-28 27-29 31-32 31-36 32-33 33-34
34-35 35-36 35-37 36-39 37-38 38-39 39-43 40-41 40-42 43-44 45-47 47-48 49-50
49-51 51-52

exact bonds :

4-10 6-7 6-22 7-8 8-9 20-27 21-30 25-26 38-40 43-45 45-46 48-49 48-54 52-53
54-55 55-56

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:CLASS 30:CLASS 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom
38:Atom 39:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS
47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS
56:CLASS

fragments assigned product role:

containing 31

fragments assigned reactant/reagent role:

containing 1

containing 13

L1 STRUCTURE UPLOADED

=> s l1 ful

FULL SEARCH INITIATED 16:14:20 FILE 'CASREACT'

SCREENING COMPLETE - 5 REACTIONS TO VERIFY FROM

2 DOCUMENTS

100.0% DONE 5 VERIFIED

5 HIT RXNS

2 DOCS

SEARCH TIME: 00.00.01

L2 2 SEA SSS FUL L1 (5 REACTIONS)

=> d ibib abs hit 1-2

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